Figure 2. Some examples of bonds connecting three successive side-chain united atoms. (A) The open circles in the upper panel correspond to a subset of possible positions of a third side chain given that the positions of the two preceding units (solid circles) are fixed and (B) illustration of excluded volume clusters. The solid dots correspond to the three lattice points along the axis orthogonal to the displayed slice. The open circles correspond to a single point in the plane.

Figure 3. Examples of the conformational transitions employed in the Monte Carlo algorithm: (A) three examples of possible two-bond moves (the number of possibilities is much larger), (B) an example of a chain-end update, (C) an example of a three-bond move, and (D) a rigid body-like displacement of a larger portion of the model chain.

Figure 4. Explanation of geometry used for the definition of the six terms describing the sequence-specific short-range interactions.

Figure 5. Illustration of model hydrogen bond geometry. The hydrogen bonds are shown by open arrows.

Figure 6. Geometry employed in the definition of the helical bias.

Figure 7. Geometry employed in the definition of the extended, β-state bias.

Figure 8. Fold of 3fxn obtained using 20 tertiary restraints compared with the native structure. The picture has been prepared using MOLMOL[42]. The native secondary structure boundaries (helices and β-strands) have been superimposed on the predicted structure. A slight distortion of one helix (bottom right of the figure) and some distortions of the central β-sheet are noticeable.

Fig. 9. Representative structure of 4fab obtained using 16 tertiary restraints compared with the native structure.

Figure 10. Schematic illustration of a protein representation. The fragment of a detailed protein structure (main chain backbone and the side chains in thinner sticks) is shown in black. The gray sticks correspond to the virtual bonds of the model chains, connecting the centers of mass of groups of atoms consisting of side chains and alpha carbons.

Figure 11. Lattice representation of the model chain and its excluded volume. The sticks correspond to the model chain virtual bonds. Excluded volume of each model amino acid is represented by 19 points on the underlying cubic lattice with the mesh size equal to 1.45 Å. The black dots correspond to three lattice points along the axis orthogonal to the picture plane (one in the plane, one below and one above the plane). The open circles correspond to single lattice points in the picture plane.

Figure 12. A fragment of the model chain and a set of vectors **w** employed in the definition of the short-range polypeptide chain stiffness.

Figure 13. Schematic illustration of the main chain's "hydrogen bonds". Residue i is hydrogen bonded to residue j and k because the vectors $\mathbf{h}_i$ and $-\mathbf{h}_I$ connect with any of the points forming of the excluded volume clusters (the clusters are symbolically shown as large spheres) of these residues.

Figure 14. Fragment of the model template chain (shown in the black sticks) and the template tube formed by the chain of spheres. The target chain (not shown in the drawing) is allowed to move in the tube with a penalty associated with all excursion from the tube.

Figure 15. Flow chart illustrating the molecular modeling procedure described in the text.

Figure 16. Stereo drawings of the two models of plastocyanin (in gray) superimposed onto crystallographic structure 2pcy (in black). The upper panel shows the model obtained by MODELLER from the threading alignment, the lower panel shows the model obtained by the procedure described in this work. For the ease of illustration, only the alpha carbon traces are shown.

Figure 17. Stereo drawings of the two models of the cytochrome 256b (in gray) superimposed onto crystallographic structure (in black). The upper panel shows the model obtained by MODELLER from the threading alignment, the lower panel shows the model obtained by the procedure described in this work. For the ease of illustration, only the alpha carbon traces are displayed.

Figure 18. Stereo drawings of the two models of telokin (in gray) superimposed onto crystallographic structure 1tlk (in black). The upper panel shows the model obtained by MODELLER from the threading alignment, the lower panel shows the model obtained by the procedure described in this work. For the ease of illustration, only the alpha carbon traces are displayed.

Figure 19. Displacement of the model chain units during the Monte Carlo simulation as a function of the position along the chain for the aligned portion of the 256b molecule. The very stable (most of the second helix and C-terminal hairpin) regions and very mobile regions (the first helix and the central loop region) are clearly separated. This is the pattern typical for successful modeling (relatively low final RMSD from the native structure).